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Parameter Uncertainty and Variability In Evaluative Fate and Exposure Models

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The human toxicity potential, a weighting scheme used to evaluate toxic emissions for life cycle assessment and toxics release inventories, is based on potential dose calculations and toxicity factors. This paper evaluates the variance in potential dose calculations that can be attributed to the uncertainty in chemical-specific input parameters as well as the variability in exposure factors and landscape parameters. A knowledge of the uncertainty allows us to assess the robustness of a decision based on the toxicity potential; a knowledge of the sources of uncertainty allows us to focus our resources if we want to reduce the uncertainty. The potential dose of 236 chemicals was assessed. The chemicals were grouped by dominant exposure route, and a Monte Carlo analysis was conducted for one representative chemical in each group. The variance is typically one to two orders of magnitude. For comparison, the point estimates in potential dose for 236 chemicals span ten orders of magnitude. Most of the variance in the potential dose is due to chemical-specific input parameters, especially half-lives, although exposure factors such as fish intake and the source of drinking water can be important for chemicals whose dominant exposure is through indirect routes. Landscape characteristics are generally of minor importance.

KEY WORDS: Multimedia modeling; uncertainty; variability; exposure efficiency; toxicity scoring; toxics release inventory (TRI); life cycle assessment (LCA).

INTRODUCTION

Multimedia mass-balance models that simulate the partitioning, transfer, and fate of chemical pollutants in the environment are increasingly used to regulate different chemicals,[1] set cleanup standards,[2] and compare emissions.[3–5] We have used CalTOX, a spreadsheet model that integrates fate analysis and the modeling of exposure pathways to calculate human toxicity potential (HTP) values.[5,6] HTP is an indicator of potential human health impact from environmental releases of chemicals that takes into account both potential dose and toxic potency.[6,7] It has been used in life-cycle assessment (LCA)[4] and for the comparison of Toxics Release Inventory (TRI) emissions.[8] In this paper, we analyze the variance or spread in the exposure assessment component of HTP that can be attributed to the combination of uncertainty and variability of input parameters.

HTP is defined as the product of potential dose and toxic potency of a chemical, normalized by the product of potential dose and toxic potency of a reference compound. We have used benzene as a reference compound for carcinogens and toluene for chemicals with non-carcinogenic effects. The toxic potency is the cancer potency as defined by EPA (q_1*) or the inverse of the reference dose or reference concentration. The potential dose (or 'exposure constants' in Guinée *et al.*[7]) is defined as the presented

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Table IA. Input data. The numbers shown are means and coefficients of variation (CV) of the log-normal distributions that were used for the input parameter values. The CV is the standard deviation devided by the mean. For the chemical-specific data (Ia), the numbers in *italic* were derived by estimation methods contained in CalTOX, whereas the other numbers are based on reported data. Where estimation methods are used, the CV depicts the uncertainty in the relation between the derived parameter and the (primary) parameter(s) used in the estimation method, e.g. between the BCF and the kow. In the Monte Carlo analysis, this is added to the uncertainty in the primary variable.

Compound name	Name	Benzene		Chlorobenzene		DDD		DDE	
Chemical abstract number	CAS	71-43-2		108-90-7		72-54-8		72-55-9	
Molecular weight (g/mol)	MW	78.11	0.0090	112.56	0.0090	320.05	0.0090	318.05	0.0090
Octanol-water partition coefficient	Kow	150.678282	2.4 E-01	644	2.7 E-01	1349412	2.1 E-01	3949681	1.0 E+00
Melting point (K)	Tm	279	0.028	228	0.03	382.15	0.03	362.15	0.03
Vapor pressure (Pa)	VP	1.27 E+04	0.04	1.61 E+03	0.08	1.30 E-04	0.52	8.43 E-04	0.49
Solubility (mol/m^3)	S	22.5	0.06	3.80	0.22	2.89 E-04	0.54	1.71 E-04	0.96
Henry's law constant (Pa-m^3/mol)	**H-**	574	0.16	275	0.46	*0.449*	0.46	*4.92*	0.46
Diffusion coefficient in pure air (m^2/d)	Dair	0.756	0.08	0.631	0.08	0.135	0.08	0.124	0.08
Diffusion coefficient in pure water (m^2/d)	Dwater	9.63 E-05	0.25	8.55 E-05	0.25	5.79 E-05	0.25	5.91 E-05	0.25
Organic carbon partition coefficient	**Koc -**	55	0.57	228	0.46	*6.48 E+05*	1.00	8.64 E+04	0.85
Distribution coefficient, ground and root soil (L/kg)	**Kd_s-**	*0.83*	0.1	*3.42*	0.10	*9.72 E+03*	0.10	*1.30 E+03*	0.10
Distribution coefficient in vadose-zone soil (L/kg)	**Kd_v -**	*0.55*	0.1	*2.28*	0.10	*6.48 E+03*	0.10	*8.64 E+02*	0.10
Distribution coefficient in ground-water zone (L/kg)	**Kd_q -**	*0.55*	0.1	*2.28*	0.10	*6.48 E+03*	0.10	*8.64 E+02*	0.10
Distribution coefficient in sediment particles (L/kg)	**Kd_d -**	*1.10*	0.1	*4.56*	0.10	*1.30 E+04*	0.10	*1.73 E+03*	0.10
Partition coefficient in plant relative to soil concentration [kg(pFM)/kg(sFM)]	**Kps -**	3	0.38	*0.183*	4	*2.20 E-03*	4	*1.18 E-03*	4
Biotransfer factor in plants relative to contaminant air concentration (m^3[a]/kg[pFM])	**Kpa -**	0.0087	14	*0.060*	14	*7.20 E+04*	14	*1.92 E+04*	14
Biotransfer factor in milk relative to cattle-diet contaminant intake (d/L)	**Bk -**	1.61 E-06	11	*5.12 E-06*	11	*0.0107*	11	*0.031*	11
Biotransfer factor in meat relative to cattle-diet contaminant intake (d/kg)	**Bt -**	1.62 E-05	13	*1.62 E-05*	13	*0.034*	13	*0.099*	13
Biotransfer factor in eggs relative to hen-diet contaminant intake (d/kg)	**Be -**	0.0012	14	*1.02 E-04*	14	*0.214*	14	*0.626*	14
Biotransfer in breast milk relative to contaminant intake by the mother (d/kg)	**Bbmk -**	3.01 E-05	10	*1.29 E-04*	10	*0.270*	10	*0.790*	10
Bioconcentration factor in fish relative to comtaminant water concentration	**BCF -**	6.79	0.43	*30.9*	0.6	*6.48 E+04*	0.6	*1.90 E+05*	0.6
Skin permeability coefficient (cm/h)	**Kp_w -**	0.19	0.57	*0.125*	2.4	*0.48*	2.4	*1.05*	2.4
Skin-water/soil partition coefficient (L/kg)	**Km -**	1	1.37	*0.015*	1.3	*1.97 E-05*	1.3	*3.26 E-04*	1.3
Reaction half-life in air (d)	Thalf_a	5.9	1.00	16.5	1.00	4.05625	1.00	4.06	1.00
Reaction half-life in ground-surface soil (d)	Thalf_g	190	1.10	75	1.10	3.21 E+03	1.10	3.21 E+03	1.10
Reaction half-life in root-zone soil (d)	Thalf_s	190	1.20	75	1.20	3.21 E+03	1.20	3.21 E+03	1.20
Reaction half-life in the vadose-zone soil (d)	Thalf_v	243	1.00	368	1.00	5.73 E+03	1.00	5.70 E+03	1.00
Reaction half-life in groundwater zone soil (d)	Thalf_q	243	1.30	218	1.30	5.73 E+03	1.30	5.70 E+03	1.30
Reaction half-life in surface water	Thalf_w	11	1.20	109	1.20	3.21 E+03	1.20	3.365	1.20
Reaction half-life in the sediment zone (d)	Thalf_d	223	1.40	334	1.40	2.88 E+03	1.40	2.86 E+03	1.40

dose to a single individual who lives in a model environment of a specific size (10,000 km^2) that has closed systems boundary.[6] It is calculated by an integrated environmental fate and exposure model such as CalTOX. Other proposals for the relative weighting of TRI or LCA emissions often do not include exposure calculations, but just rely on toxic potency or combine toxic potency with persistence and bio-concentration factors.[6]

The need to investigate the uncertainty in environmental impact evaluation for life-cycle assessment[9–13] and toxic release evaluation[14] has been widely recognized, but is only now being addressed.

Huijbregts[15] has proposed a general framework for uncertainty analysis in LCA that is very specific to the types of uncertainty that occur in LCA. He has also suggested ways to investigate the covariance between different LCA results in order not to overestimate the uncertainty. Steen[16] has presented an uncertainty analysis for the Environmental Priority System, an alternative impact assessment method that is based on economic damage calculations. To illustrate the role of uncertainty calculations in decision making, Steen has applied this uncertainty analysis to a hypothetical case.

Our effort is based on a framework for the analysis of uncertainty in human health risk assessment developed by Finkel.[17] It distinguishes between parameter uncertainty, model uncertainty, decision rule uncertainty, and natural variability in any of the pa-

Table IA. (*Continued*)

Name	Fluoranthene		Lindane		Isophorone		Nitrobenzene		Tetrachloroethylene		Toluene		Vinyl chloride	
CAS	206-44-0		58-89-9		78-59-1		98-95-3		127-18-4		108-88-3		75-01-4	
MW	202.26	0.0090	290.85	0.0090	138.2	0.0090	123.11	0.0090	165.8	0.0090	92.13	0.0090	62.5	0.009
Kow	127092	2.8 E-01	5288	3.2 E-01	50	6.0 E-02	69	1.3 E-01	382	2.0 E-01	482	2.3 E-01	15	6.9 E-01
Tm	384.15	0.03	385.65	0.028	265.05	0.03	279	0.03	252	0.028	178	0.03	119	0.028
VP	1.19 E-03	0.45	6.15 E-03	0.62	55.3	0.18	33	0.15	2563	0.06	3769	0.02	101300	0.09
S	1.16 E-03	0.14	0.0176	0.51	86.8	0.39	16	0.05	1.73	0.50	6.22	0.32	39	0.31
H -	*1.02*	0.46	*0.35*	0.46	*0.64*	0.46	*2.11*	0.46	1459	0.14	663	0.46	2567	0.13
Dair	0.261	0.08	0.152	0.08	0.54	0.08	0.66	0.08	0.66	0.05	0.75	0.08	0.914	0.05
Dwater	5.90 E-05	0.25	5.51 E-05	0.25	6.66 E-05	0.25	8.93 E-05	0.25	8.82 E-05	0.25	8.51 E-05	0.25	1.21 E-04	0.25
Koc -	4.94 E+04	0.11	1.50 E+03	0.40	*24*	1.00	156	0.56	197	0.60	139	0.33	29	1.36
Kd_s -	*741.495*	0.10	*22.485*	0.10	*0.36*	0.10	*2.34*	0.10	*2.95*	0.1	*2.085*	0.10	*0.44*	0.1
Kd_v -	*494.33*	0.10	*14.99*	0.10	*0.24*	0.10	*1.56*	0.10	*1.97*	0.1	*1.39*	0.10	*0.29*	0.1
Kd_q -	*494.33*	0.10	*14.99*	0.10	*0.24*	0.10	*1.56*	0.10	*1.97*	0.1	*1.39*	0.10	*0.29*	0.1
Kd_d -	*988.66*	0.10	*29.98*	0.10	*0.48*	0.10	*3.12*	0.10	*3.94*	0.1	*2.78*	0.10	*0.58*	0.1
Kps -	*8.64 E-03*	4	*0.054*	4	*0.803*	4	*0.666*	4	0.23	4	*0.22*	4	1.45	4
Kpa -	*2.97 E+03*	14	*364*	14	*3.38*	14	*1.24*	14	0.01	14	*0.0194*	14	1.03 E-03	14
Bk -	*1.01 E-03*	11	*4.2E-05*	11	*3.97 E-07*	11	*5.48 E-07*	11	3.12 E-06	10.8	*3.83 E-06*	11	3.80 E-07	10.8
Bt -	*3.19 E-03*	13	*1.33 E-04*	13	*1.26 E-06*	13	*1.73 E-06*	13	2.75 E-05	12.6	*1.21 E-05*	13	4.72 E-06	12.6
Be -	*2.01 E-02*	14	*8.38 E-04*	14	*7.92 E-06*	14	*1.09 E-05*	14	3.03 E-03	14	*7.64 E-05*	14	1.21 E-04	14
Bbmk -	*2.54 E-02*	10	*1.06 E-03*	10	*1.00 E-05*	10	*1.38 E-05*	10	7.63 E-05	10	*9.64 E-05*	10	3.03 E-06	10
BCF -	*6.10 E+03*	0.6	*254*	0.6	*2.4*	0.6	*3.31*	0.6	44.3	0.15	*23*	0.6	10	1
Kp _w -	*1*	2.4	*0.014*	2.4	*1.43 E-02*	2.4	*1.98 E-02*	2.4	0.049	2.4	*0.111*	2.4	0.812	2.4
Km -	*5.41 E-04*	1.3	*2.51 E-04*	1.3	*1.58 E-02*	1.3	*3.39 E-03*	1.3	1	0.27	*0.021*	1.3	1	0.27
Thalf_a	0.463	1.00	2.1175	1.00	7.38 E-02	1.00	3	1.00	51	1.00	2.375	1.00	3.22	1.00
Thalf_g	852	1.10	152	1.10	18	1.10	61	1.10	594	1.10	28	1.10	278	1.10
Thalf_s	852	1.20	152	1.20	18	1.20	61	1.20	594	1.20	28	1.20	278	1.20
Thalf_v	1020	1.00	123	1.00	63	1.00	196	1.00	760	1.00	109	1.00	260	1.00
Thalf_q	580	1.30	123	1.30	35	1.30	196	1.30	515	1.30	18	1.30	4349	1.30
Thalf_w	1.74	1.20	127	1.20	18	1.20	105	1.20	25	1.20	13	1.20	1351	1.20
Thalf_d	950	1.40	209	1.40	60	1.40	100	1.40	515	1.40	107	1.40	1114	1.40

rameters. Finkel calls for a separate treatment of the different types of uncertainty, because—depending on the purpose of the analysis—different tools will be used to analyze the different types of uncertainty. Cost-effective measures of uncertainty reduction differ among sources of uncertainty.

METHODS

The uncertainty in life-cycle impact assessment and especially the robustness and reliability of the toxicity evaluations have become key concerns in the LCA community.[10,18] Our analysis addresses two questions related to the robustness and reliability of toxicity evaluations.

One, how large is the typical variance in potential dose calculations? A knowledge of the typical spread is important for decision making, because it allows us to assess the robustness of the decision[16] and the likelihood of recommending an inferior alternative in a comparative assessment or of focusing on unimportant aspects of the product life-cycle. Uncertainty estimates have been used to conduct switch-point analyses, which investigate how much a single parameter or group of parameters has to change to reverse the recommendation of an LCA. This creative approach allows for the assessment of decision-confidence when selecting from a finite number of alternatives.[19]

Two, when is it advisable to calculate site specific or geographically differentiated HTP values? Another way of asking this question is: How large is the potential error caused by not knowing where the emissions occur, which is usually the case in LCA. Several authors have argued that it is necessary to conduct site specific assessments of toxic impacts in LCA in order to account for differences in landscape

parameters.[10] To answer this question we compare the importance of the variability in landscape parameters, the variability in exposure conditions, and the uncertainty in chemical specific input parameters.

The present analyses makes use of the CalTOX model (Version 2.2) as modified for the calculation of toxic equivalency potentials.[4] CalTOX, a risk assessment model, integrates a multimedia environmental fate model with a multiple pathway exposure model.[20] The CalTOX modifications have been described by Hertwich *et al.*[5,6]

The most general way to define exposure is in terms of a concentration of a specified contaminant in a specified medium and the time that the receptor has contact with that medium. In the most general sense, an exposure assessment involves the quantification of a link among a source of contamination, its transport and transformation among a set of environmental media, and human contact with exposure media.[22–25] Environmental media include outdoor air, indoor air, ground-surface soil, root-zone soil, plants, ground water, and surface water in a contaminated landscape, as well as carpets, furnishings, etc., in indoor environments. Exposure media include substances with which we have direct contact such as outdoor air, indoor air, food, household dust, homegrown foods, animal food products, and tap water. An exposure pathway defines the link between an environmental medium and exposure medium for inhalation, ingestion, and dermal uptake routes of exposure. Potential dose, expressed as average daily dose, is the amount of material per unit of body weight per day (mg/kg-d) that enters the lungs (inhalation route), enters the gastrointestinal tract (ingestion route), or crosses into the stratum corneum (dermal-contact route).[22,24] For HTP, a route-specific estimate of potential dose is combined with a measure of inherent, route-specific toxicity (i.e., cancer potency, reference dose) for a risk-based scaling of chemicals.[7]

Multimedia models can be used to provide a screening level assessment of source to exposure/dose relationship of regional emissions. The most widely used multimedia models are the mass-conservative Mackay-type compartment models.[26–29] These models are most appropriate for treating transport and transformation of chemicals emanating from non-point sources over relatively long time and length scales at low concentrations. The various media, represented by compartments, are assumed to be individually well mixed. Transport between compartments occurs in response to gradients in chemical fugacity or concentration. Multimedia models have been used successfully for modeling the transport and transformation of nonionic organic chemicals in complex environmental systems[28] and linking chemical transport to human exposure.[21]

HTP calculations use multimedia fate and exposure models to calculate ''exposure constants,'' which represent the potential dose received by an individual living in the model environment as a result of a unit release of 1 kg/day.[6,7] This is similar to the concepts of exposure efficiency or potential dose effectiveness,[30,31] but it does not include differences in population density. In addition, HTP calculations are conducted in a closed system: the entire life-cycle of a pollutant is considered in the assessment, not only the time spent near the release site. Exposure is accounted for without regard to whether the exposed person lives close to or far from the facility.[6,32] This is an important analytical choice and may not be appropriate for some purposes, e.g. environmental justice assessments. According to our classification, the question of open vs. closed systems boundaries and, in the case of open boundaries, the selection of a proper model-system size represent decision-rule uncertainties.

The Monte Carlo analysis software package, Crystal Ball™ 4.2 was used to carry out variance propagation and to assess uncertainty importance.[33] The input data used for this analysis consists of three different data sets: chemical-specific data, exposure factors data, and landscape data. These data are summarized in Tables Ia, Ib, and Ic. All input parameters were assumed to be log-normally distributed. The means and coefficients of variation for these distributions are also presented in Tables Ia, Ib, and Ic. For each chemical in the original CalTOX data set, the Cal-EPA has prepared either its own report or made use of existing Cal-EPA reports to summarize and evaluate the measured and estimated value ranges of chemical-specific inputs.[34] In this analysis, the values, ranges, and distributional characteristics of chemical-specific parameters were derived from the primary literature. The supporting Cal-EPA and U.S. EPA reports contain a detailed bibliography of the literature references and the statistical methods used to assess measures of central tendency and measures of

[4] The CalTOX model and documentation[21] can be downloaded from http://www.cwo.com/~herd1/downset.htm, and the necessary modifications are available from the corresponding author. The use of CalTOX for HTP calculations is described in http://www.scorecard.org/env-releases/def/tep_gen.html.

Table IB: Exposure Factors

Exposure factors		Mean	CV
Body weight (kg)	BW	62.1	0.2
Surface area (m^2/kg)	SAb	0.026	0.07
Active breathing rate (m^3/kg-h)	BRa	0.019	0.3
Resting breathing rate (m^3/kg-h)	BRr	0.0064	0.2
Fluid intake (L/kg-d)	Ifl	0.022	0.2
Fruit and vegetable intake (kg/kg-d)	Ifv	0.0049	0.2
Grain intake (kg/kg-d)	Ig	0.0037	0.2
Milk intake (kg/kg-d)	Imk	0.0065	0.2
Meat intake (kg/kg-d)	Imt	0.003	0.2
Egg intake (kg/kg-d)	Iegg	0.00046	0.3
Fish intake (kg/kg-d)	Ifsh	0.00029	2
Soil ingestion (kg/kg-d)	Isl	0.00000035	3
Breast milk ingestion by infants (kg/kg-d)	Ibm	0.11	0.2
Inhalation by cattle (m^3/d)	Inc	122	0.3
Inhalation by hens (m^3/d)	Inh	2.2	0.3
Ingestion by pasture by dairy cattle (kg[FM]/d)	Ivdc	85	0.2
Ingestion of pasture by beef cattle (kg[FM]/d)	Ivbc	60	0.4
Ingestion of pasture by hens (kg[FM]/d)	Ivh	0.12	0.04
Ingestion of water by dairy cattle (L/d)	Iwdc	35	0.2
Ingestion of water by beef cattle (L/d)	Iwbc	35	0.2
Ingestion of water by hens (L/d)	Iwh	0.084	0.1
Ingestion of soil by cattle (kg/d)	Isc	0.4	0.7
Ingestion of soil by hens (kg/d)	Ish	0.000013	1
Fraction of water needs provided by ground water	fw_gw	0.5	0.5
Fraction of water needs provided by surface water	fw_sw	0.5	0.5
Fraction of water contaminants transferred to soil by irrigation	f_ir	0.25	1
Fraction of fruits and vegetables that are exposed produce	fabv_grd_v	0.47	0.1
Fraction of fruits and vegetables local	flocal_v	1	0
Fraction of grains local	flocal_g	1	0
Fraction of milk local	flocal_mk	1	0
Fraction of meat local	flocal_mt	1	0
Fraction of eggs local	flocal_egg	1	0
Fraction of fish local	flocal_fsh	1	0
Plant-air partition factor for particles, m^3/kg[FM]	Kpa_part	3300	1.8
Rainsplash rate constant {(mg/kg[plnt FM])/(mg/kg[soil])}	rainsplash	0.0034	1
Water use in the shower (L/min)	Wshower	8	0.4
Water use in the house (L/h)	Whouse	40	0.4
Room ventilation rate, bathroom (m^3/min)	VRbath	1	0.4
Room ventilation rate, house (m^3/h)	VRhouse	750	0.3
Exposure time, in shower or bath (h/day)	ETsb	0.27	0.6
Exposure time, active indoors (h/day)	ETai	15	0.4
Exposure time, outdoors at home (h/day)	ETao	1	0.4
Exposure time, indoors resting (h/day)	ETri	8	0.04
Indoor dust load (kg/m^3)	dust_in	0.00000003	0.4
Exposure frequency to soil on skin, (d/y)	EFsl	137	0.6
Soil adherence to skin (mg/cm^2)	Slsk	0.5	0.4
Ratio of indoor gas conc. to soil gas conc.	alpha_inair	0.0001	2
Exposure time swimming (h/d)	ETsw	0.5	0.5
Exposure frequency, swimming (d/y)	EFsw	15	4
Water ingestion while swimming (L/kg-h)	Isww	0.0007	1
Exposure duration (years)	ED	80	0.15
Averaging time (days)	AT	25550	0.1

Table IC: Landscape Data

Landscape properties		Mean	CV
Contaminated area in m^2	Area	1.00E+10	0.1
Annual average precipitation (m/d)	rain	0.0011	1
Flux; surface water into landscape (m/d)	inflow	0	0.1
Land surface runoff (m/d)	runoff	0.000275	1
Atmospheric dust load (kg/m^3)	rhob_a	6.15E-08	0.2
Deposition velocity of air particles (m/d)	v_d	500	0.3
Plant dry mass inventory ($kg[DM]/m^2$)	bio_inv	0.7	0.2
Plant dry-mass fraction	bio_dm	0.2	0.2
Plant fresh-mass density kg/m^3	rho_p	1000	0.2
Ground-water recharge (m/d)	recharge	0.00012	1
Evaporation of water from surface water (m/d)	evaporate	0.00028	1
Thickness of the ground soil layer (m)	d_g	0.01	1
Soil particle density (kg/m^3)	rhos_s	2600	0.05
Water content in surface soil (volume fraction)	beta_g	0.1	0.2
Air content in the surface soil (volume fraction)	alpha_g	0.17	0.2
Erosion of surface soil (kg/m^2-d)	erosion_g	0.0003	0.2
Thickness of the root-zone soil (m)	d_s	2	0.2
Water content of root-zone soil (volume fraction)	beta_s	0.28	0.2
Air content of root-zone soil (volume fraction)	alpha_s	0.17	0.2
Thickness of the vadose-zone soil (m)	d_v	5	0.1
Water content; vadose-zone soil (volume fraction)	beta_v	0.28	0.2
Air content of vadose-zone soil (volume fraction)	alpha_v	0.17	0.2
Thickness of the aquifer layer (m)	d_q	3	0.3
Solid material density in aquifer (kg/m^3)	rhos_q	2600	0.05
Porosity of the aquifer zone	beta_q	0.2	0.2
Fraction of land area in surface water	f_arw	0.00815	0.2
Average depth of surface waters (m)	d_w	5	1
Suspended sediment in surface water (kg/m^3)	rhob_w	0.8	1
Suspended sediment deposition ($kg/m^2/d$)	deposit	10.5	0.3
Thickness of the sediment layer (m)	d_d	0.05	1
Solid material density in sediment (kg/m^3)	rhos_d	2600	0.05
Porosity of the sediment zone	beta_d	0.2	0.2
Sediment burial rate (m/d)	bury_d	0.000001	5
Ambient environmental temperature (K)	Temp	288	0.02
Surface water current in m/d	current_w	0	1
Organic carbon fraction in upper soil zone	foc_s	0.015	1
Organic carbon fraction in vadose zone	foc_v	0.01	1
Organic carbon fraction in aquifer zone	foc_q	0.01	1
Organic carbon fraction in sediments	foc_d	0.02	1
Boundary layer thickness in air above soil (m)	del_ag	0.005	0.2
Yearly average wind speed (m/d)	v_w	0.01	1

variance and spread (range and/or standard deviation). In the development of supporting data for CalTOX, estimation methods were used to estimate chemical parameters for which there are few or no literature values.[35] For chemicals analyzed in this paper, we have used CalEPA's authorized data set and Cal-EPA procedures for dealing with chemicals not included in the current data set.[36] Based on current Cal-EPA practice, the coefficients of variation for known chemicals have been applied to similar chemicals in situations where only limited data are available.[36] The variability in landscape parameters reflects the variability in the state of California as summarized by Schwalen *et al.*[37] It is currently used by Cal-EPA for landfill assessments.[36] The variability in exposure parameters was derived from EPA's exposure factors handbook.[38] These are also the values currently used by Cal-EPA.[36]

This analysis builds on the development of HTP values for a total of 236 chemicals presented in Hertwich *et al.*[5] For each chemical and each release medium, the most important exposure route was identified. Chemicals were grouped by dominant exposure route. For each exposure route, a representative chemical was selected that was fairly well characterized in terms of the data available and that had a typical

potential dose and persistence. Figure 1 displays the ranges of potential dose in each exposure group, the number of chemicals, and the chemical selected in this paper to represent each group. Monte Carlo analysis was used to propagate the variance in the model input parameters and thus determine the variance of the potential dose. Monte Carlo simulations were conducted for each selected chemical to address the uncertainty in chemical-physical parameters alone, as well as the uncertainty in these parameters in conjunction with the variability in landscape and exposure parameters. The joint analysis of uncertainty and variability included a sensitivity analysis that identified the contribution-to-variance by different input parameters. Sensitivity analysis is an optional output of Crystal Ball.[33] This sensitivity analysis was used to evaluate the relative contribution to variance of the different input parameter sets. The contribution-to-variance was then compared with the difference in the variance between Monte Carlo simulations of the uncertainty in chemical-physical parameters alone and of the joint uncertainty and variability.

RESULTS

The calculated exposure distributions are displayed in Fig. 2. Table II presents the statistics for the distributions. The results reveal that the uncertainty of the dose estimate—as defined by the ratio of the 95th to the 5th percentile—is typically about one order of magnitude, although it varies from 1/2 to 3-1/2 orders of magnitude. The uncertainty is higher for chemicals that have significant indirect exposure routes and higher for air emissions than for surface water emissions. The figure also shows the distribution of dose estimates among all chemicals modeled, which spans about 6–7 orders of magnitude (5th to 95th percentile).

In Table II we also compare the statistics of

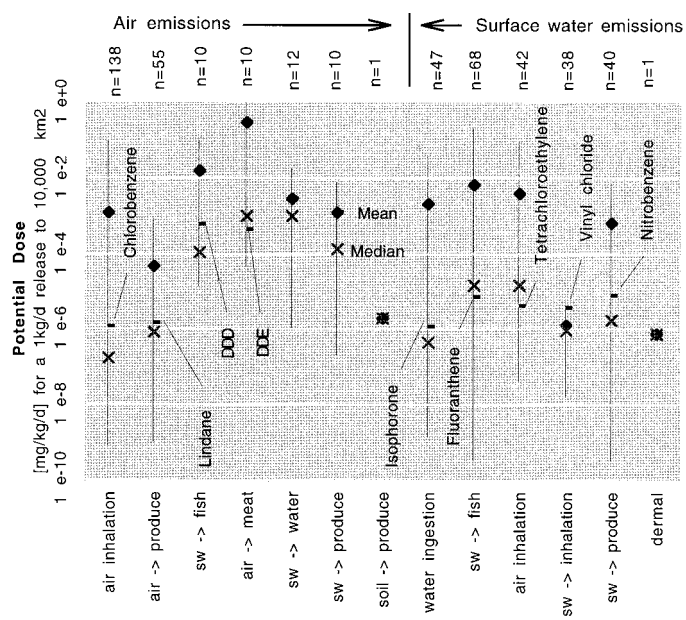

Fig. 1. Distribution of potential dose estimates calculated by CalTOX in a 10,000 km^2 environment with closed systems boundaries and California landscape characteristics. The lines represent the range of potential dose estimates (minimum to maximum) for chemicals grouped by dominant exposure route. The mean and the median for the group, as well as the point estimate for that chemical of the group for which uncertainty analysis was conducted, are indicated on the graph. n refers to the number of chemicals in each group. Representative chemicals were selected from the smaller input data set provided by CalEPA; probabalistic data was not available for the others. Hence, four exposure routes could not be modelled.

potential dose calculations for simulations with and without landscape and exposure variability. The comparison shows that, for air emissions, the magnitude of variance is very similar between the two. For surface water emissions, the inclusion of landscape and exposure variability increases the degree of variance somewhat, in the case of vinyl chloride significantly.

The results of the sensitivity analysis are shown in Fig. 3. For all chemicals except vinyl chloride, the contribution of the uncertainty in chemical-specific parameters to the variance in HTP is larger than the contribution from the variability in other parameters. For air emissions, chemical-specific parameters dominate the total variance, whereas for surface water emissions the variability in exposure parameters can have a substantial contribution to the total variance. The contribution of the variability in landscape parameters is always 10% or less. Table III lists the most important parameters contributing to exposure variance for each chemical. It shows an interesting pattern: the persistence of the chemical in the release compartment is the most important parameter for all the surface water emissions other than vinyl chloride, as well as the chemicals with direct inhalation as their most important exposure route (benzene, chlorobenzene, toluene). For DDD and DDE, the biotransfer from air to plants is most important. For surface water emissions, the source of drinking water is important, because surface water receives direct emissions whereas the effect on ground water is very indirect. We are exposed to chemicals contained in drinking water either through direct ingestion of the water or through the inhalation of chemicals evaporated off shower water. In addition, chemicals contained in irrigation water may enter the food supply.

DISCUSSION

In this section, we consider the impact of our findings on life cycle impact assessment. We address two issues, the potential for uncertainty analysis to guide the design of an impact assessment scheme, and the implications of the sensitivity analysis, especially the high contribution-to-variance of exposure parameters, for the scoring of toxic chemicals.

The Monte Carlo analysis shows that the 90% confidence interval due to chemical specific uncertainty lies somewhere between a factor of 3 and a factor of 100, with only one outlier (DDE). Figure 1

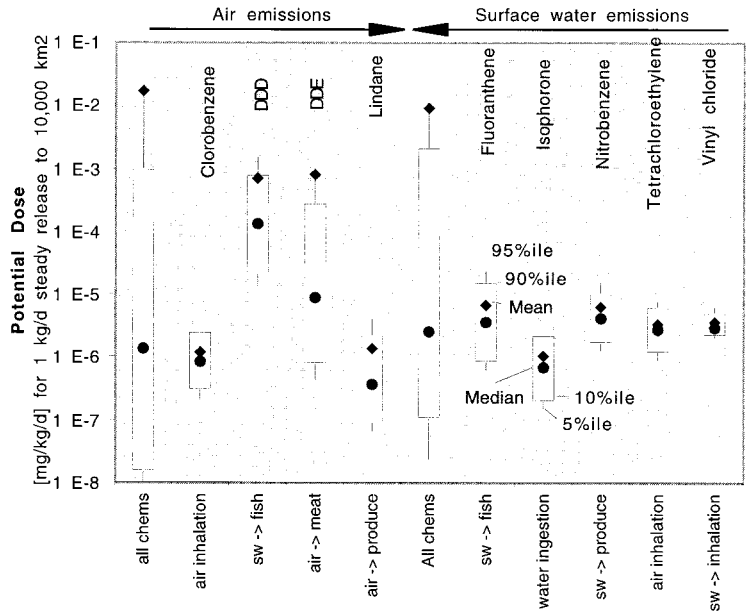

Fig. 2. The variance in potential dose of the selected chemicals as determined by Monte Carlo simulations. Only the uncertainty in chemical specific parameters was taken into account. The graph also lists the most important exposure route for each of the chemicals. 'All chems' labels the variation of potential dose point estimates among 236 chemicals

Table II. Statistical measures of dose received by an adult individual in the Monte Carlo simulations of representative chemicals considering only the uncertainty in chemical-specific parameters (no var), as well as including the variability in landscape and exposure parameters (var). SD represents the standard deviation and GSD the geometric standard deviation (= SD of the logarithm) 95%/15% represents the ratio of the 95th percential to the 5th percentile.

		Chlorobenzene air inhalation		DDD sw → fish		DDE sw → meat		Lindane air → produce		Toluene air inhalation		Benzene air inhalation	
AIR	All chems	var	no var	var	no var	var	no var	var	no var	var	no var	var	no var
Percentiles:													
5%	1.0 E-8	2.0 E-7	2.2 E-7	6.9 E-6	1.3 E-5	3.8 E-7	5.1 E-7	5.7 E-8	1.2 E-7	2.8 E-8	3.0 E-8	7.2 E-8	7.7 E-8
10%	1.5 E-8	2.7 E-7	2.9 E-7	1.3 E-5	2.2 E-5	6.5 E-7	8.4 E-7	8.1 E-8	1.6 E-7	3.7 E-8	4.0 E-8	9.8 E-8	1.0 E-7
90%	9.9 E-4	2.5 E-6	2.5 E-6	1.4 E-3	8.1 E-4	2.8 E-4	3.0 E-4	2.4 E-6	4.0 E-6	3.6 E-7	3.5 E-7	8.9 E-7	8.7 E-7
95%	9.9 E-3	3.4 E-6	3.2 E-6	2.7 E-3	1.5 E-3	7.8 E-4	8.5 E-4	4.8 E-6	7.4 E-6	4.9 E-7	4.8 E-7	1.2 E-6	1.2 E-6
Mean:	1.6 E-2	1.2 E-6	1.2 E-6	8.6 E-4	6.8 E-4	9.3 E-4	8.5 E-4	1.4 E-6	2.4 E-6	1.7 E-7	1.7 E-7	4.3 E-7	4.3 E-7
Median:	1.4 E-6	8.2 E-7	8.4 E-7	1.3 E-4	1.3 E-4	9.0 E-6	9.8 E-6	3.4 E-7	6.3 E-7	1.2 E-7	1.2 E-7	2.9 E-7	3.1 E-7
SD:	1.9 E-1	1.2 E-6	1.2 E-6	1.2 E-2	1.8 E-2	2.7 E-2	2.0 E-2	8.1 E-6	1.8 E-5	1.8 E-7	1.7 E-7	4.6 E-7	4.4 E-7
GSD	1.9	0.38	0.36	0.79	0.63	1.03	1.01	0.59	0.56	0.38	0.36	0.37	0.36
95%/5%	960000	17	15	396	117	2041	1673	85	63	18	16	17	15

		Fluoroanthene sw → fish		Isophorone water ingestion		Nitrobenzene sw → produce		Tetrachloro-ethylene air inhalation		Vinyl chloride sw → inhalation	
SW	All chems	var	no var	var	no var	var	no var	var	no var	var	no var
Percentiles:											
5%	2.3 E-8	1.5 E-7	5.8 E-7	5.3 E-8	1.5 E-7	3.8 E-7	1.3 E-6	7.3 E-7	9.1 E-7	5.9 E-7	2.1 E-6
10%	1.1 E-7	2.7 E-7	8.5 E-7	1.2 E-7	2.0 E-7	8.8 E-7	1.7 E-6	1.0 E-6	1.2 E-6	1.1 E-6	2.2 E-6
90%	2.1 E-3	1.7 E-5	1.5 E-5	2.5 E-6	2.2 E-6	1.1 E-5	9.9 E-6	6.8 E-6	6.0 E-6	6.7 E-6	4.9 E-6
95%	1.1 E-2	3.3 E-5	2.3 E-5	3.6 E-6	3.1 E-6	1.7 E-5	1.5 E-5	8.7 E-6	7.7 E-6	8.9 E-6	6.4 E-6
Mean:	9.0 E-3	8.0 E-6	6.5 E-6	1.1 E-6	1.0 E-6	7.2 E-6	6.1 E-6	3.5 E-6	3.4 E-6	3.8 E-6	3.5 E-6
Median:	2.6 E-6	2.1 E-6	3.5 E-6	6.5 E-7	6.9 E-7	3.7 E-6	4.1 E-6	2.7 E-6	2.8 E-6	2.9 E-6	2.9 E-6
SD:	8.0 E-2	2.5 E-5	9.1 E-6	1.9 E-6	1.4 E-6	6.4 E-5	1.3 E-5	3.6 E-6	2.5 E-6	5.9 E-6	3.0 E-6
GSD	1.77	0.7	0.48	0.59	0.4	0.51	0.33	0.33	0.28	0.37	0.16
95%/5%	493721	219	39	68	21	43	12	12	9	15	3

		Toluene sw → inhalation		Benzene water ingestion	
SW	All chems	var	no var	var	no var
Percentiles:					
5%	2.3 E-8	1.5 E-7	2.7 E-7	1.6 E-7	3.5 E-7
10%	1.1 E-7	2.3 E-7	3.7 E-7	2.7 E-7	4.8 E-7
90%	2.1 E-3	2.3 E-6	1.8 E-6	3.2 E-6	2.6 E-6
95%	1.1 E-2	3.0 E-6	2.1 E-6	4.4 E-6	3.1 E-6
Mean:	9.0 E-3	1.1 E-6	1.1 E-6	1.6 E-6	1.4 E-6
Median:	2.6 E-6	8.8 E-7	9.4 E-7	1.1 E-6	1.3 E-6
SD:	8.0 E-2	1.2 E-6	7.6 E-7	2.0 E-6	8.9 E-7
GSD	1.77	0.41	0.28	4.4 E-1	2.9 E-1
95%/5%	493721	20	8	28	8.9

indicates the point estimates of potential dose for the 236 chemicals that have been assessed in Hertwich *et al.*[5] span a range of 10 orders of magnitude (Table II indicates that the 90% range of potential dose point estimates spans 6–7 orders of magnitude). This means that the potential dose calculations for these fairly well defined chemicals offer a significant information gain.

The analysis indicates that we have sufficient information to justify the use of potential dose calculations in the assessment of chemicals. We do not have to resort to simpler models such as those proposed by Jia *et al.*[14] At the same time, we suggest that proposals for the use of more complex models or indicators, such as site-specific assessments or damage calculations based on epidemiological data, are also tested with respect to their informativeness.

Table III. Contribution-to-variance (in percent) of different input parameters in the sensitivity analysis. Exposure parameters are in *ital,* landscape parameters in **bold.** No more than 5 parameters are shown; the balance to 100% is "other parameters."

air	
Benzene	
Reaction half-life in air	91.6
Active breathing rate	*7.2*
Resting breathing rate	*0.1*
Chlorobenzene	
Reaction half-life in air	90.5
Active breathing rate	*8.0*
Resting breathing rate	*0.2*
Exposure time, indoor resting	*0.1*
DDD	
Air-plant biotransfer factor	27.7
Fish intake	*22.3*
Reaction half-life in air	10.3
Reaction half-life in ground-surface soil	5.3
Vapour pressure	4.6
DDE	
Air-plant biotransfer factor	47.2
Octanol-water partition coefficient	20.2
Reaction half-life in air	11.3
Solubility	5.0
Biotransfer factor in milk relative to cattle-diet contaminant intake	3.7
Lindane	
Reaction half-life in air	41.5
Air-plant biotransfer factor	27.3
Vapour pressure	4.8
Fish intake	*3.2*
Solubility	3.0
Toluene	
Reaction half-life in air	90.7
Active breathing rate	*8.5*
surface water	
Fluoroanthene	
Fish intake	*44.7*
Reaction half-life in surface water	35.0
Bioconcentration factor in fish relative to contaminant water concentration	8.0
Organic carbon fraction in sediments	**3.2**
Suspended sediment in surface water	**3.1**
Isophorone	
Reaction half-life in surface water	67.9
Fraction of water needs provided by ground water	*22.0*
Fraction of land area in surface water	**2.9**
Partition coefficient in plant relative to soil concentration	1.5
Fluid intake	*0.9*
Nitrobenzene	
Reaction half-life in surface water	38.6
Fraction of water needs provided by ground water	*31.6*
Partition coefficient in plant relative to soil concentration	8.5
Fraction of land area in surface water	**5.5**
Exposure time, in shower or bath	*2.4*
Tetrachloroethylene	
Reaction half-life in surface water	39.9
Reaction half-life in air	35.9
Fraction of water needs provided by ground water	*7.1*
Active breathing rate	*7.0*
Fish intake	*2.8*
Toluene	
Reaction half-life in surface water	51.3
Fraction of water needs provided by ground water	*23.2*
Fraction of land area in surface water	**4.7**
Exposure time, in shower or in bath	*3.7*
Fish intake	*2.8*
Vinyl chloride	
Fraction of water needs provided by ground water	*45.7*
Exposure time, in shower or in bath	*12.6*
Fraction of land area in surface water	**10.3**
Skin permeability coefficient	*9.1*
Active breathing rate	*5.0*
Benzene	
Reaction half-life in surface water	47.8
Fraction of water needs provided by ground water	*23.5*
Organic-carbon content of surface soil	**5.5**
Fraction of irrigation water contaminants transferred to soil	*4.5*
Fraction of land area in surface water	**3.6**

The findings of the sensitivity analysis are both interesting and surprising. For most chemicals, the uncertainty in what we know about the chemical properties contributes more to the variance in potential dose than the variability in exposure factors and landscape properties. There is little difference in the ratio of the 95th to 5th percentile between calculations that include exposure and landscape variability and those that do not. The effect of variation in landscape properties, even in a state as diverse as California, is small compared to the effect of variation in breathing rates, fish consumption, and the source of drinking water. This is corroborated by a comparison of HTP values for different landscapes representing the contiguous 48 U.S. states.[39]

Some researchers and decision makers have criticized the use of generic assessments in LCA and pointed to the importance of differences in landscape characteristics.[10] They call for site specific exposure modeling, or at least for a geographical differentia-

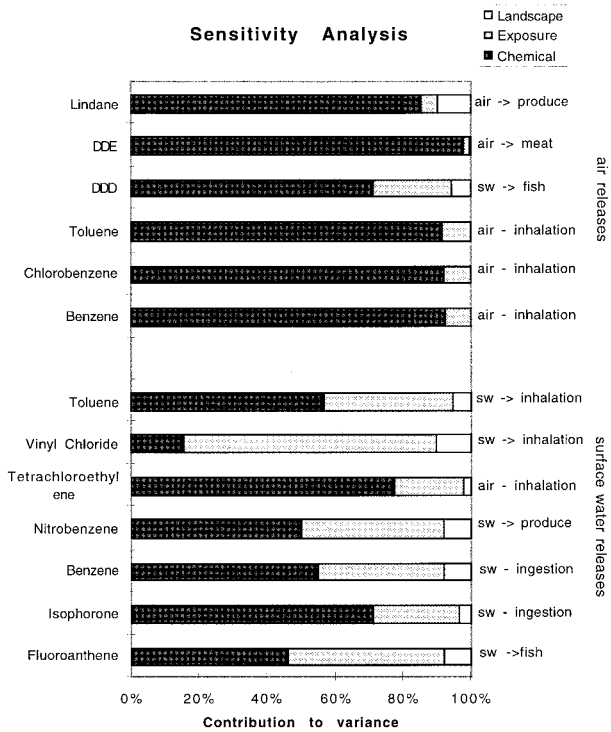

Fig. 3. Contribution-to-variance of different data sets. "Chemical" refers to chemical-specific data, "landscape" to landscape data used for fate and transport modeling, and "exposure" to data concerning exposure routes (e.g., source of drinking water, and contact rates).

tion of the effects of toxic emissions at the regional level. Our investigation indicates that the effect of the variance in landscape parameters will in many cases not be significant once the variance in other parameters has been taken into account. The variance in potential dose does not increase significantly when the variance in landscape specific parameters is included (Table II), and the contribution of landscape parameters to the overall variance is usually less than 10%. If the overall form of the HTP is accepted, the use of a generic set of HTP values is justified and efforts to improve exposure assessment should focus on a better characterization of chemical parameters.

The importance of exposure parameters especially for surface water releases poses a problem to the design of the impact assessment method. Should the scoring system be designed to protect the average person, or should it protect highly exposed individuals, such as populations with a high fish consumption or people who drink a lot of tap water that is produced from surface water? We could choose to conduct a Monte Carlo analysis for each chemical and then use the 95th or 99th percentile as the basis of the comparison, not a point estimate. In fact, a point estimate is likely to reward chemicals with high uncertainty or large exposure variability because the point estimate is more likely to be close to the median than to the expected value (mean), and the mean tends to be higher than the median especially for lognormal distributions with a large spread. The use of probabilistic calculations for developing HTP scores depends on our ability to characterize and quantify the uncertainty in all our input parameters. Such an approach is hampered by the lack of systematic data collection and verification efforts for chemical-specific parameters.

CONCLUSIONS

In this paper, we show that the parameter uncertainty in potential dose is typically 1/2 to 2 orders of magnitudes, but it can be as large as 3 1/2 orders of magnitudes. The uncertainty in exposure is hence smaller than or comparable to the uncertainty in the toxicity of the chemicals. We have shown that despite the remaining uncertainty, fate and exposure modeling offers a means to narrow down the uncertainty in potential dose from an initial six orders of magnitudes to one order, a significant gain in information. The sensitivity analysis shows that uncertainty in chemical-specific data is more important than the variability of landscape and exposure parameters. We recommend that efforts to improve potential dose calculations focus on a better characterization of chemical-specific parameters.

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